Overview of Modeling and Simulation
TCAD - FLOOPS / FLOODS

Gator Engineering
University of Florida

Outline

- Modeling Overview
  - Strain Effects
  - Thermal Modeling
- TCAD Modeling
  - FLOOPS / FLOODS Introduction
  - Progress on GaN Devices
  - Prospects for Reliability Simulation

Self-consistent Procedure

- k•p self-consistent solution to Poisson and Schrödinger's equation

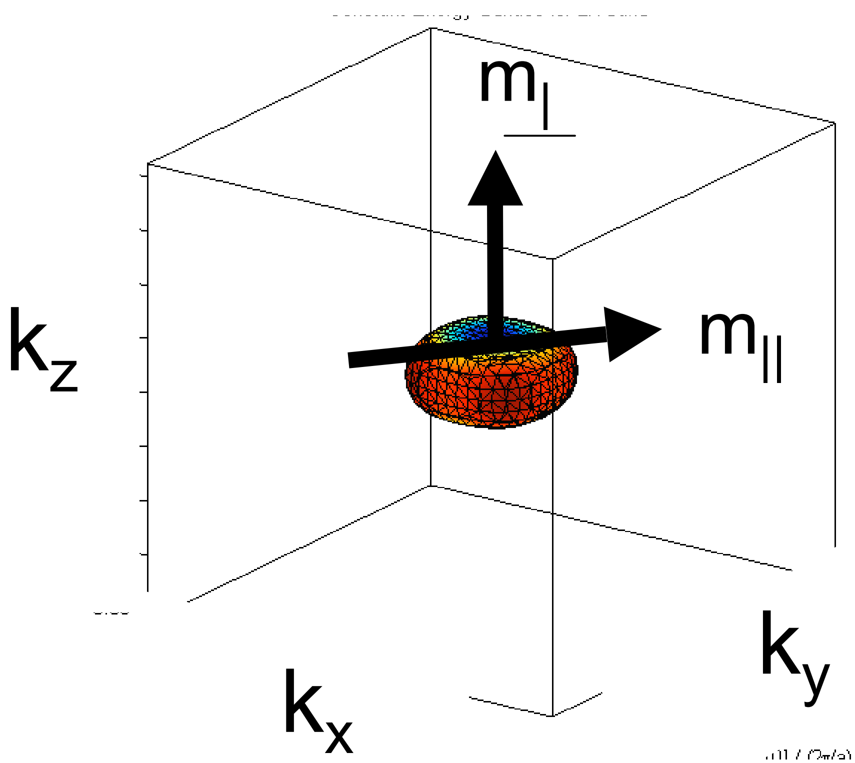
$$-\frac{d^2}{dz^2}V(z) = q/\varepsilon_{Si}[N(z) + N_D(z)]$$

$$[\frac{P^2}{2m} + V(z)]\Psi_n(z) = E\Psi_n(z)$$

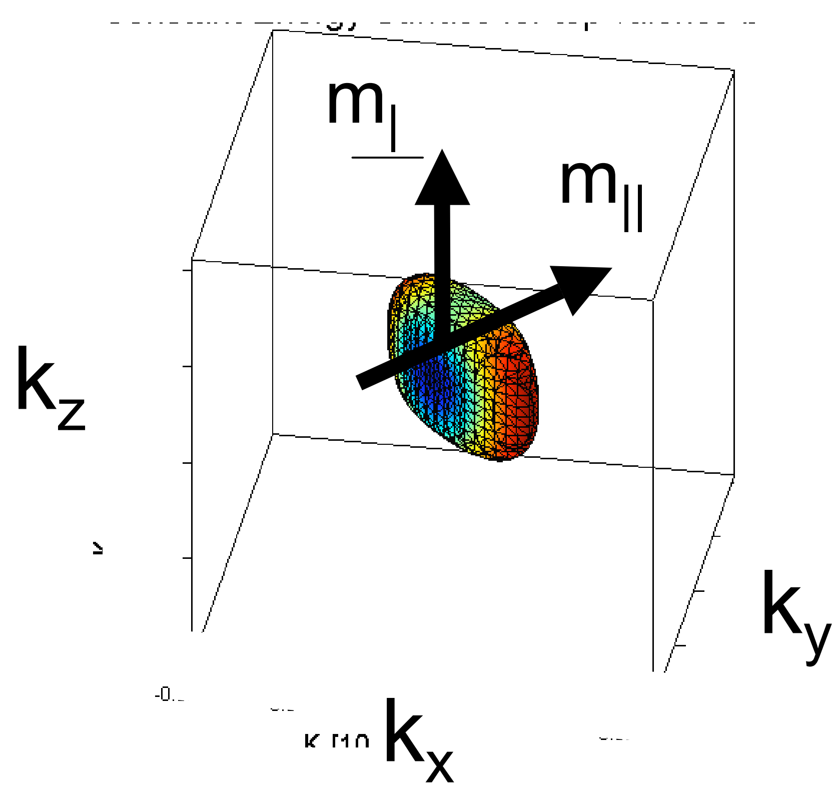
$$N(z) = 2\sum_n |\Psi_n(z)|^2 f_{2D}(E)$$

In and Out-of-Plane Masses (Ge)

Biaxial Stress



Uniaxial Stress

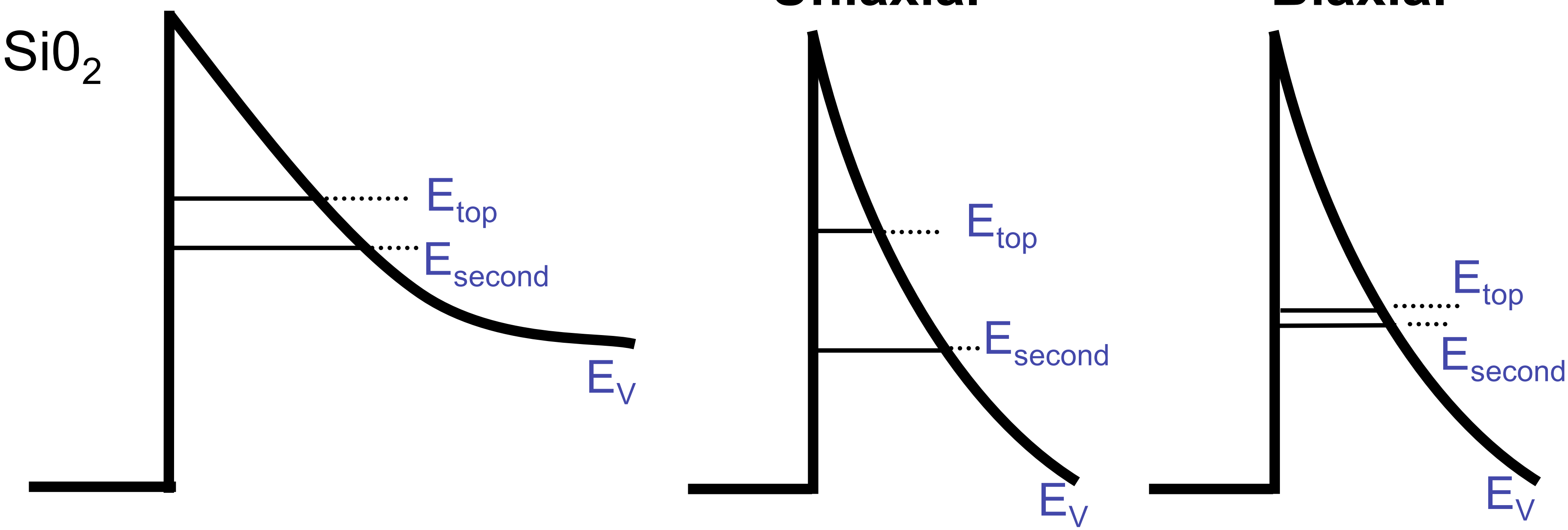


Using k•p methods to compute bands

Confinement and Strain Sub-band Shifts

High Vertical Field

Low Vertical Field **Uniaxial** **Biaxial**

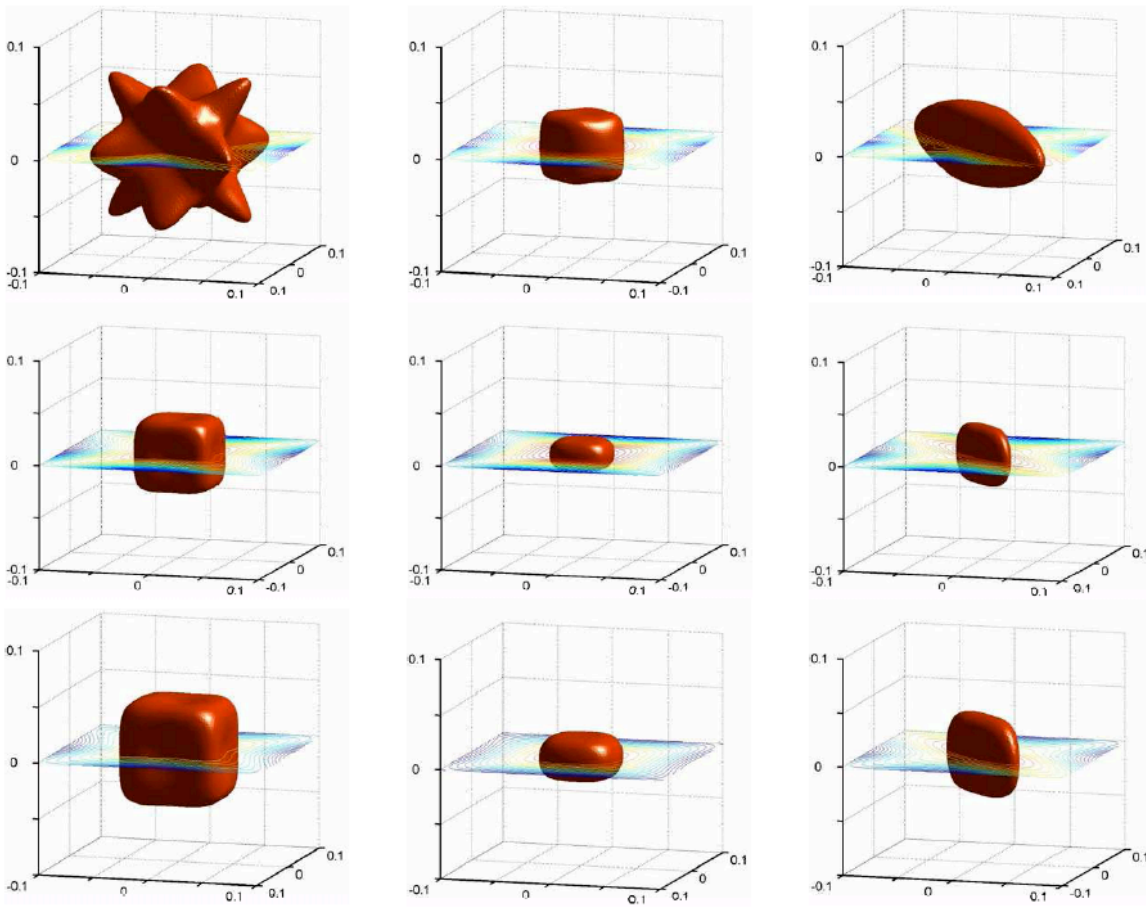


Band splitting due to strain

Splitting (increases) / (decreases)

under confinement

Same Physics for IV, III-V Materials



Si

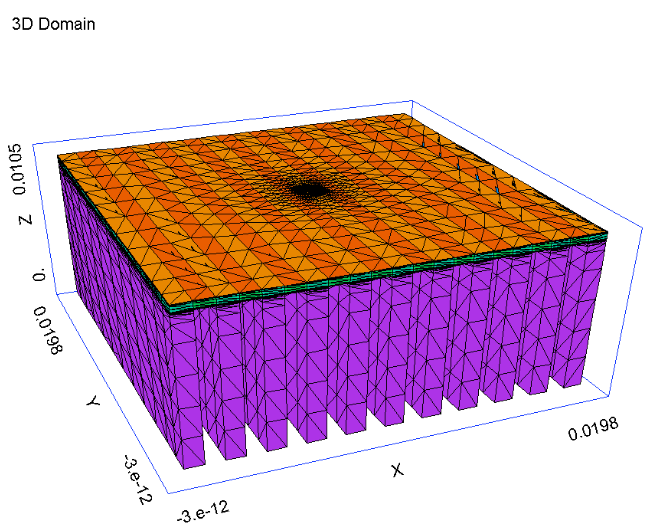
Ge

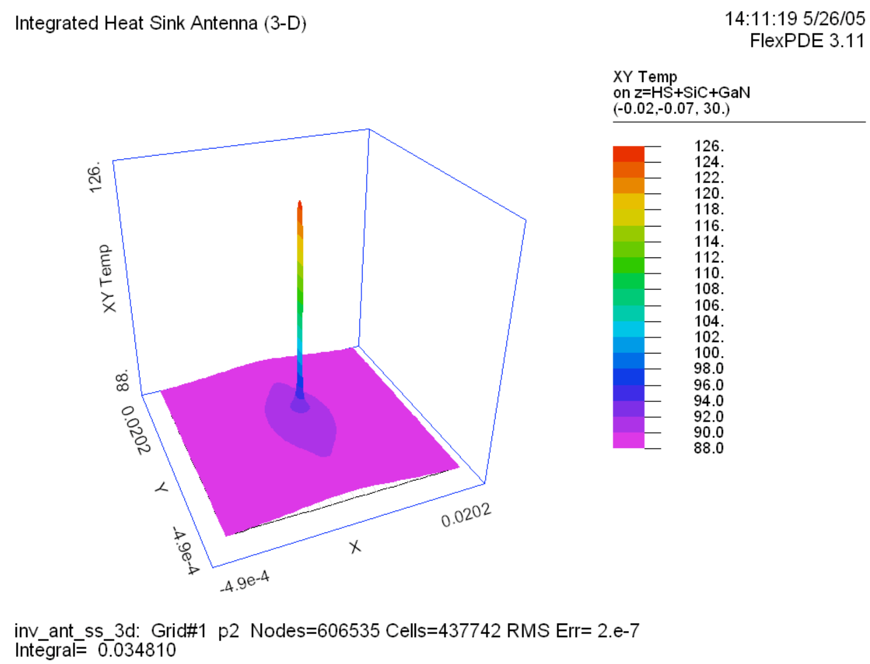
GaAs

Unstressed   1GPa Biaxial Tension   1GPa Uniaxial Compression

Thermal Simulations

- Use finite element modeling to optimize package design
- Most important factors in thermal management: heat transfer at the system boundaries and substrate thickness
- Couple w/ FLOOPS / FLOODS simulations as well

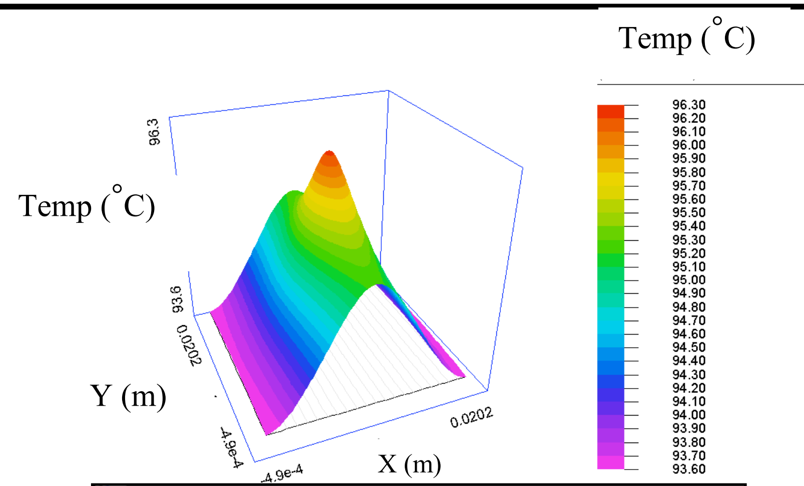


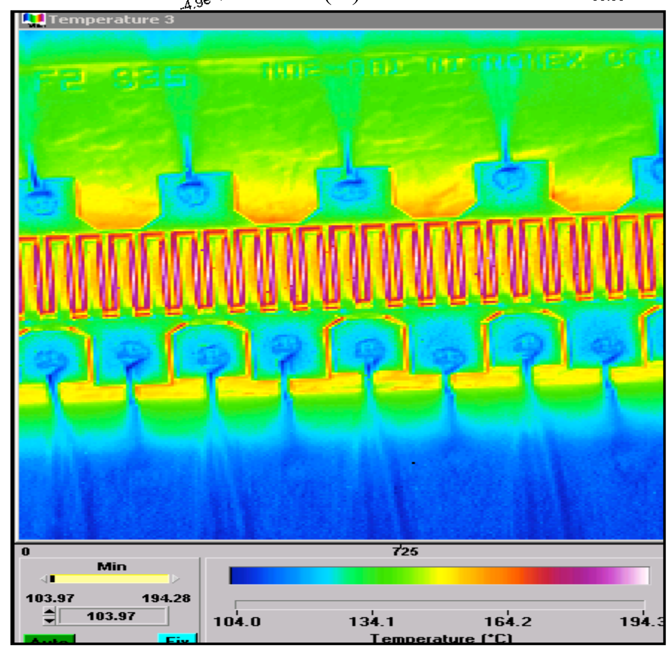


Thermal Simulations and IR Imaging

- T(Junc) of power devices is often significantly hotter than T(stage)
- Accurate extraction of activation energy requires knowledge of the true channel temperature.
- We have extensive experience in estimating heat transfer even in complex structures
- Purchasing a high-resolution IR camera for direct imaging of the device operating temperature. We have collaborated with Nitronex on thermal imaging-a typical example is shown at right for a multi-finger power HEMT.

- Possible Collaborations w/ Samuel Graham, Georgia Tech





Outline

- Modeling Overview
  - Strain Effects
  - Thermal Modeling
  - TCAD Based Approaches
- TCAD Modeling
  - FLOOPS / FLOODS Introduction
  - Progress on GaN Devices
  - Prospects for Reliability Simulation

FLOOPS / FLOODS

- Object-oriented codes
- Multi-dimensional
- P = Process / D = Device 90% code shared
- Scripting capability for PDE's - Alagator

- Commercialized - ISE / Synopsis
  - Sentaurus - Process is based on FLOOPS
- Licensed at over 300 sites world-wide
  - 2008 release
  - Manual is online (but needs updating)

What is Alagator?

- Scripting language for PDE's
- Parsed into an expression tree
- Assembled using FV / FE techniques
- Stored in hierarchical parameter data base

- Models are accessible, easily modified

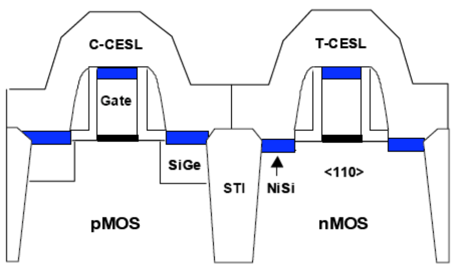
What is Alagator?

Operator	*Description*
"ddt"	Time derivative
"grad"	Spatial derivative
"sgrad"	Scharfetter / Gummel Discretization Operator
"dot"	Returns the dot product of the gradient of two field – electric field in direction of current floq
"elastic"	Compute elastic forces - FEM balance

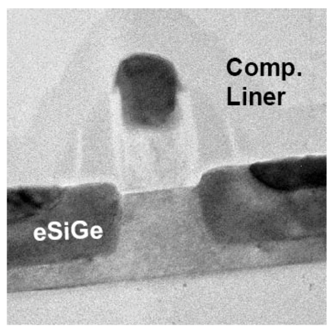
- Example use of operators for diffusion equation
- Fick's Second Law of Diffusion
  - ddt(Boron) - 9.0e-16 * grad(Boron) - K * (Boron - Trap)
  - $\partial C(x,t) / \partial t = D \partial^2 C(x,t) / \partial x^2$

Strained PMOS

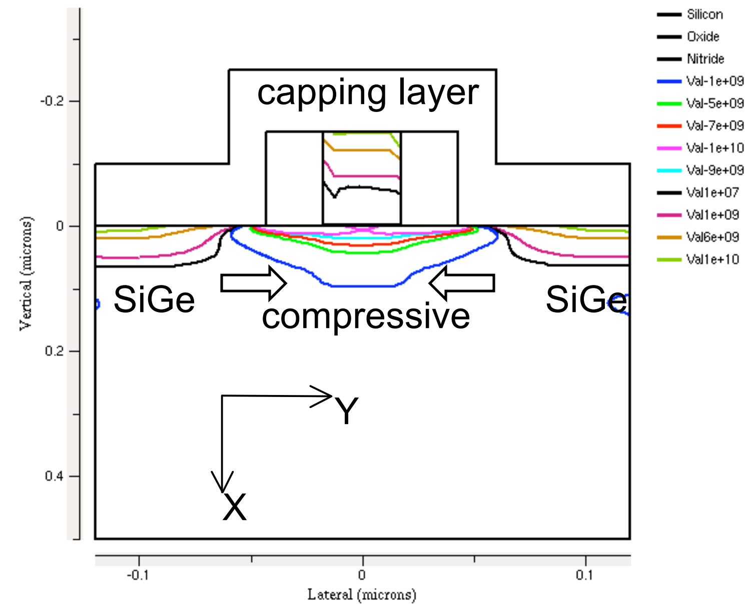
- To enhance channel mobility, PMOS strain processing includes embedded SiGe in the source/drain regions and compressive capping layers.
- FLOOXS predicts strain/stress profiles where the channel stress is ~1 GPa



Cheng, *et al.* IEDM 2007

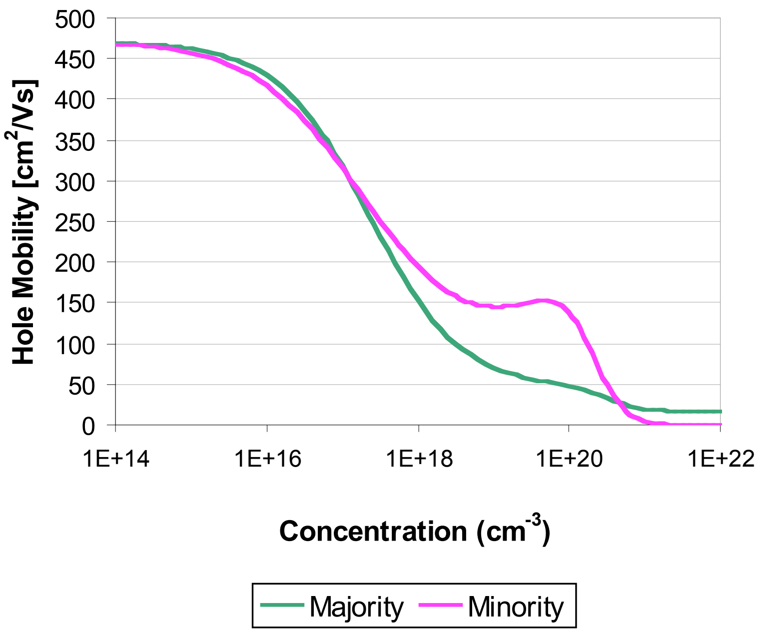


Horstmann, *et al.* IEDM 2005



FLOOXS predicted stress profile [dyne/cm2]
(YY component - channel direction)

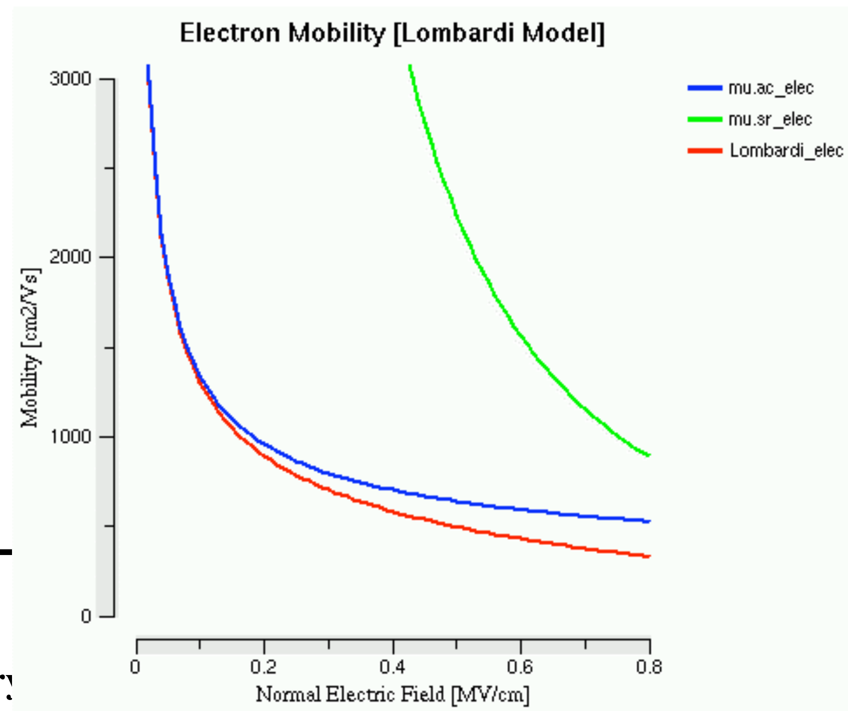
Complex Mobility Models Construction



Unifies the description of majority and minority carrier bulk mobilities

- temperature dependence
- electron–hole scattering
- screening of ionized impurities by carriers
- clustering of impurities

Surface scattering terms (Vertical Field)
Velocity Saturation
EffMass changes w/ strain (more later)

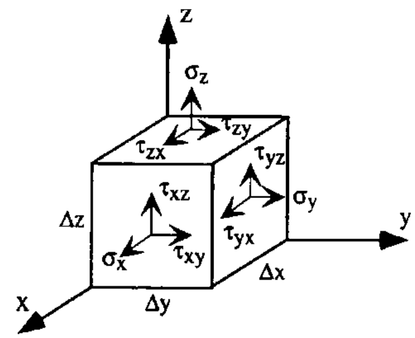


Piezoresistance

- Piezoresistivity is the change in electrical resistivity with mechanical stress and involves the relationships between electric field E_i, current density J_j, and mechanical stress σ_{kl}

$$E_i = \left(\rho_{ij} + \Pi_{ijkl}\sigma_{kl}\right)J_j$$

(Small Change Limit)



$$\underbrace{\begin{bmatrix} -\Delta\mu_{xx}/\mu_{xx} \\ -\Delta\mu_{yy}/\mu_{yy} \\ -\Delta\mu_{zz}/\mu_{zz} \\ -\Delta\mu_{yz}/\mu_{yz} \\ -\Delta\mu_{zx}/\mu_{zx} \\ -\Delta\mu_{xy}/\mu_{xy} \end{bmatrix}}_{\text{Mobility Change}} = \underbrace{\begin{bmatrix} \Delta\rho_{xx}/\rho_{xx} \\ \Delta\rho_{yy}/\rho_{yy} \\ \Delta\rho_{zz}/\rho_{zz} \\ \Delta\rho_{yz}/\rho_{yz} \\ \Delta\rho_{zx}/\rho_{zx} \\ \Delta\rho_{xy}/\rho_{xy} \end{bmatrix}}_{\text{Resistivity Change}} = \underbrace{\begin{bmatrix} \pi_{11} & \pi_{12} & \pi_{12} & 0 & 0 & 0 \\ \pi_{12} & \pi_{11} & \pi_{12} & 0 & 0 & 0 \\ \pi_{12} & \pi_{12} & \pi_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \pi_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \pi_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \pi_{44} \end{bmatrix}}_{\text{Piezoresistance coefficients}} \underbrace{\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{bmatrix}}_{\text{Stress components}}$$

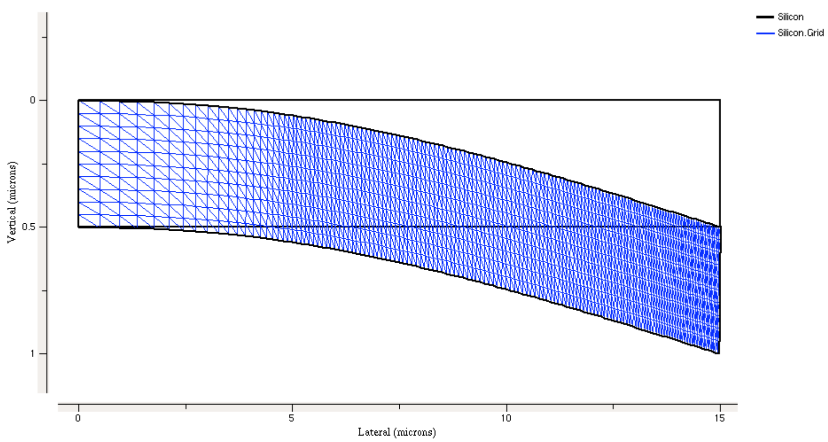
$$J_{n,p} = -qn\mu_{n,p}\nabla\phi_{n,p}$$

$$\begin{bmatrix} J_X(\sigma) \\ J_Y(\sigma) \\ J_Z(\sigma) \end{bmatrix} = \begin{bmatrix} 1-\Delta\mu_{xx}/\mu_{xx} & -\Delta\mu_{xy}/\mu_{xy} & -\Delta\mu_{zx}/\mu_{zx} \\ -\Delta\mu_{xy}/\mu_{xy} & 1-\Delta\mu_{yy}/\mu_{yy} & -\Delta\mu_{yz}/\mu_{yz} \\ -\Delta\mu_{zx}/\mu_{zx} & -\Delta\mu_{yz}/\mu_{yz} & 1-\Delta\mu_{zz}/\mu_{zz} \end{bmatrix} \begin{bmatrix} J_X(0) \\ J_Y(0) \\ J_Z(0) \end{bmatrix}$$

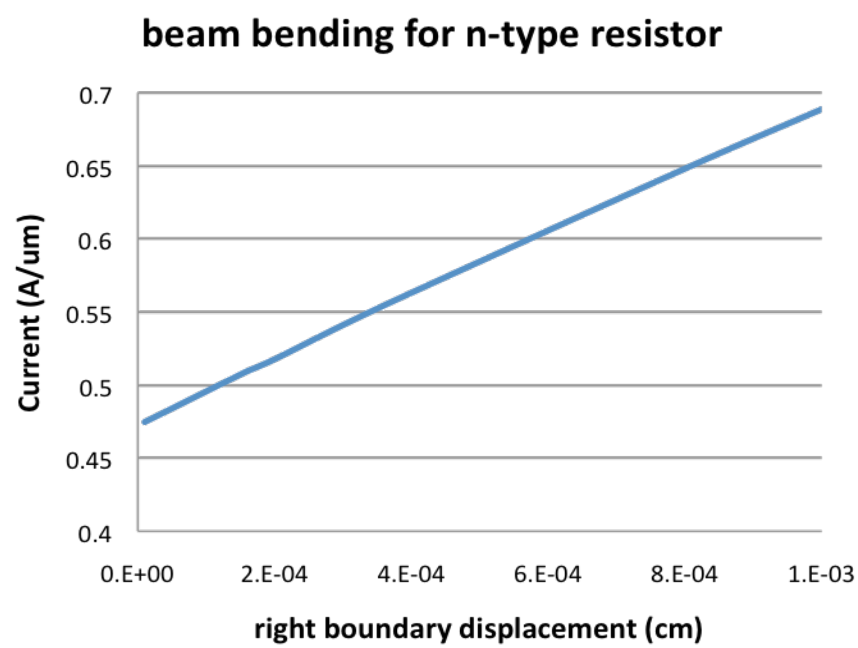
Piezoresistance example

- Silicon beam with an n-type surface
- Bending induces tensile stress at the surface resulting in a increase in mobility and current.

$$J_X(\sigma) \cong \left(1 + \frac{-\Delta\mu_{xx}}{\mu_{xx}}\right) J_X(0) = \left(1 + \pi_{11}\sigma_{xx}\right) J_X(0)$$



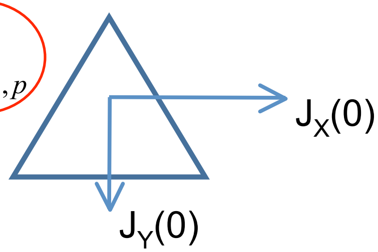
FLOOXS beam bending example



Piezoresistance

- The gradient of the quasi-fermi level gives $J_{n,p}$ vector values for each element

$$J_{n,p} = -qn\mu_{n,p}\nabla\phi_{n,p}$$

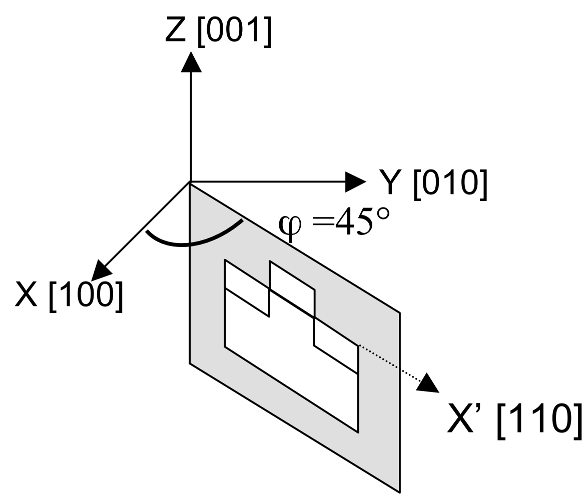


$$\begin{bmatrix} J_X(\sigma) \\ J_Y(\sigma) \end{bmatrix} = \begin{bmatrix} 1-\Delta\mu_{xx}/\mu_{xx} & -\Delta\mu_{xy}/\mu_{xy} \\ -\Delta\mu_{xy}/\mu_{xy} & 1-\Delta\mu_{yy}/\mu_{yy} \end{bmatrix} \begin{bmatrix} J_X(0) \\ J_Y(0) \end{bmatrix}$$

- Piezoresistance coefficient matrix can be defined for any orientation using directional cosines

$$\pi_{ijkl}' = \sum_m \sum_n \sum_o \sum_p a_{mi} a_{nj} a_{ok} a_{pl} \pi_{mnop}$$

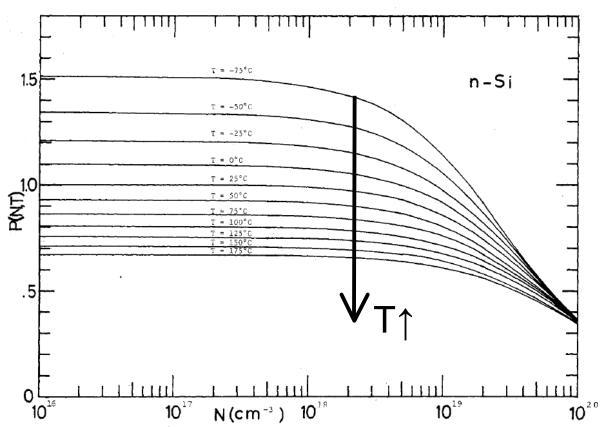
$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} \cos\phi\cos\theta & -\sin\phi & \cos\phi\sin\theta \\ \sin\phi\cos\theta & \cos\phi & \sin\phi\sin\theta \\ -\sin\theta & 0 & \cos\theta \end{bmatrix}$$



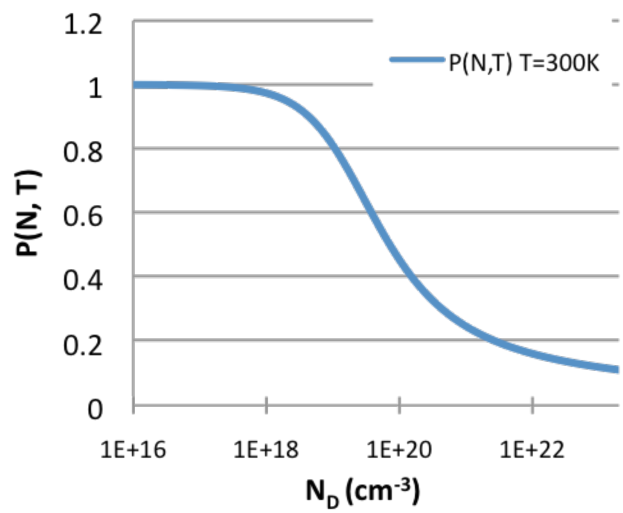
Piezoresistance

- Piezoresistance coefficients can be set to spatially vary in FLOODS
  - Extracted channel and bulk coefficients different (to do)
- Piezoresistance coefficients are function of impurity concentration and temperature P(N,T)

$$P_{n,p}(N,T) = \frac{300}{T}\frac{F'_{s+(1/2)}\left(E_{F_{n,p}}/(k_B T)\right)}{F_{s+(1/2)}\left(E_{F_{n,p}}/(k_B T)\right)}$$



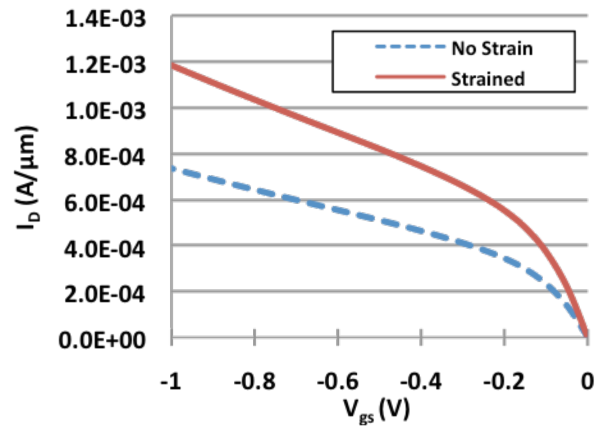
Kanda Y., IEEE Trans Electron Devices 1987

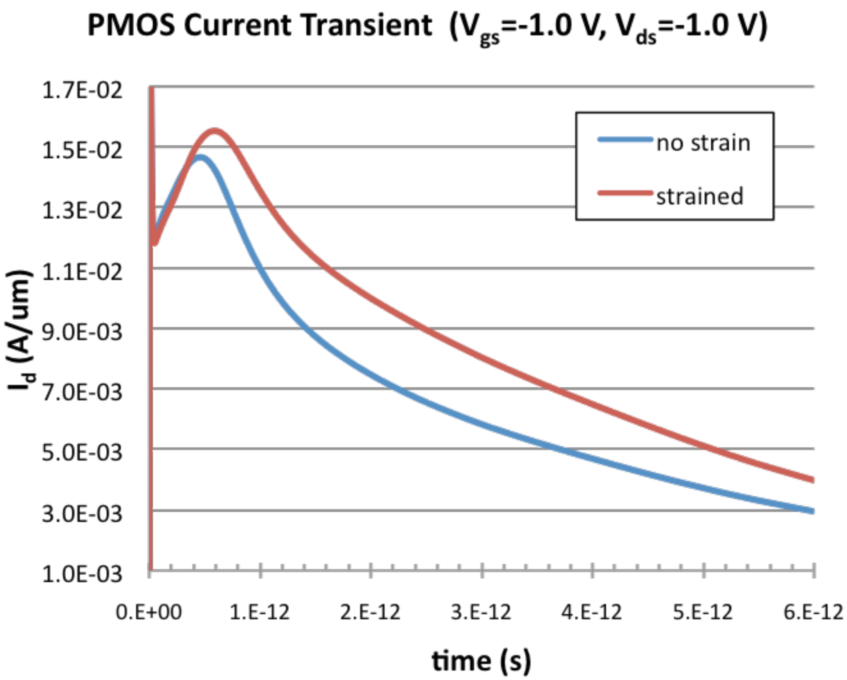


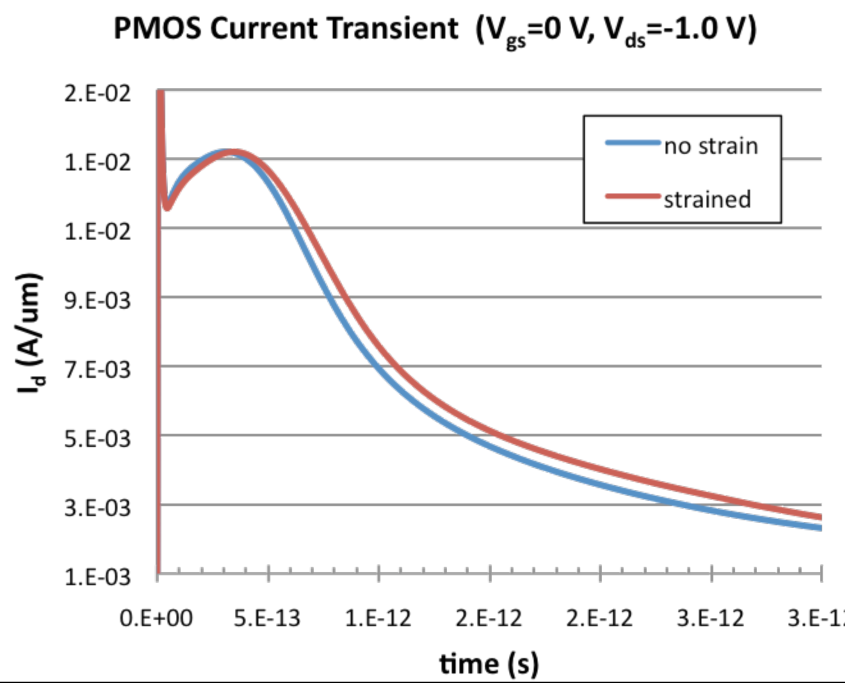
FLOODS simulated piezoresistance factor for T=300 K

Strained PMOS Simulations

- PMOS with L_{gate}=30 nm
- <110> channel orientation
- 2007 ITRS dimensions
- Charge strike dist. in drain

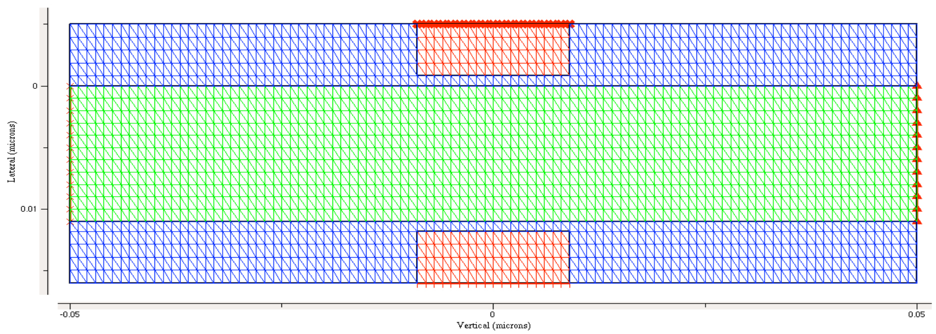




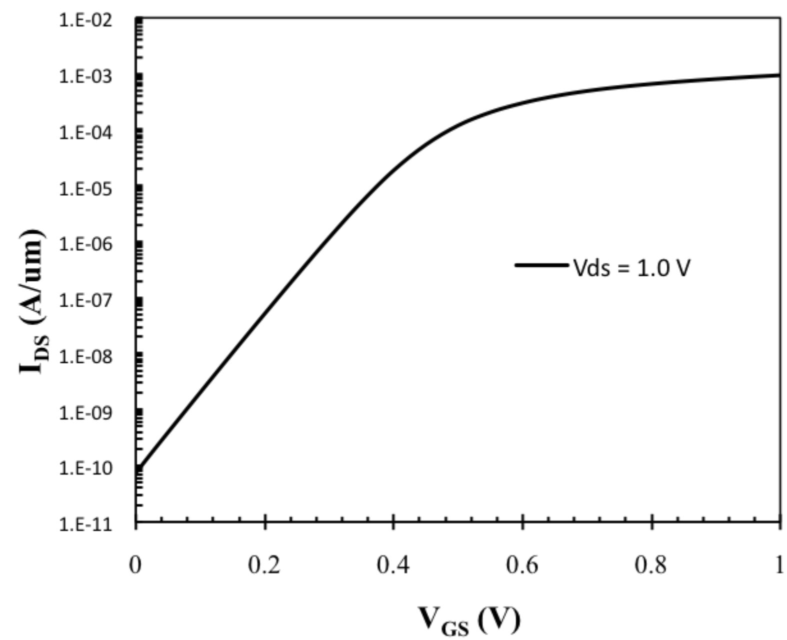


Double-Gate FinFET

- L_{gate}=18 nm, w_{si}=11 nm
- Midgap metal gate (typically TiN)
- Gate-S/D doping underlap to control V_t and short channel effects
- Undoped body



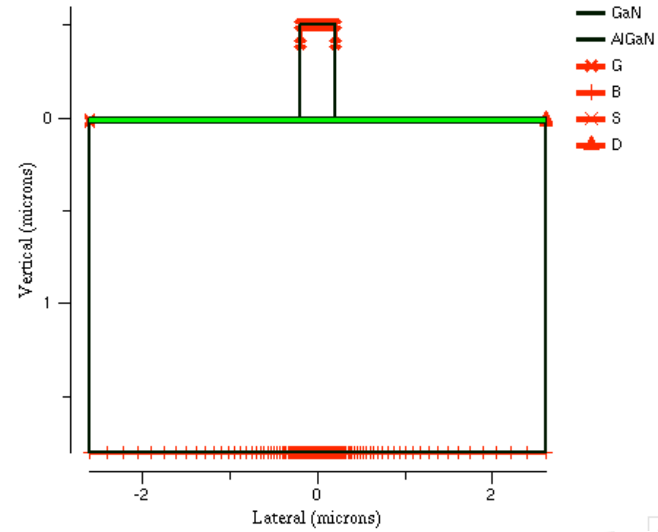
FinFET top cross-sectional view

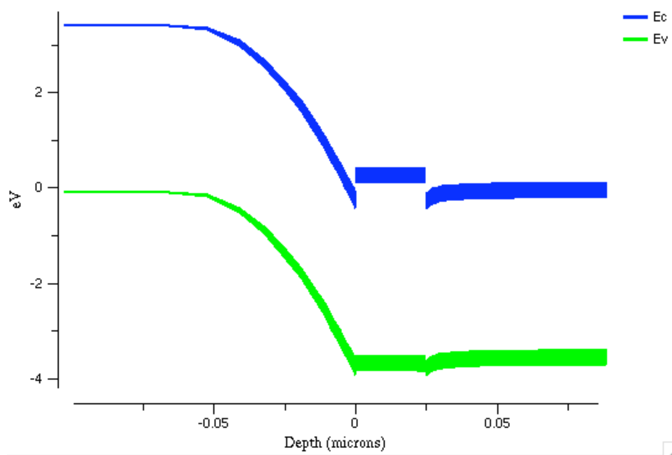


nFinFET I-V characteristic

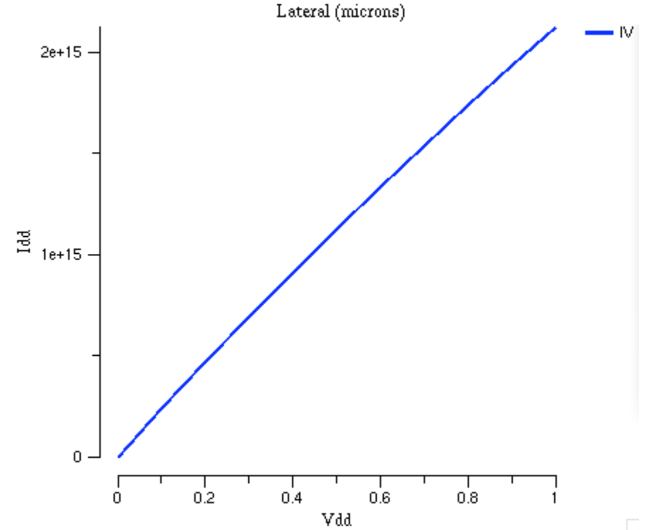
AlGaN/GaN HEMT Device

- Can handle heterostructure bands
- Gate offsets
- Field Dependence



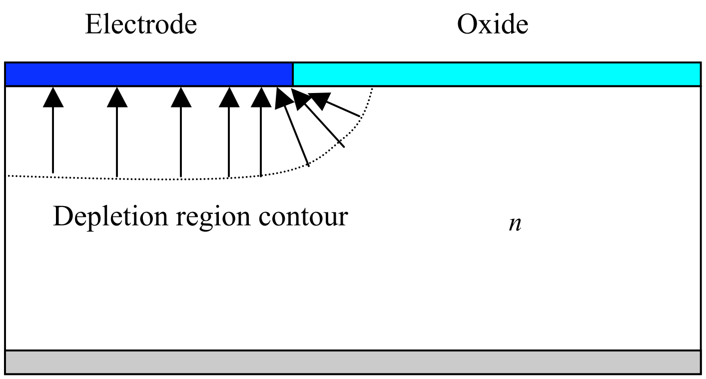


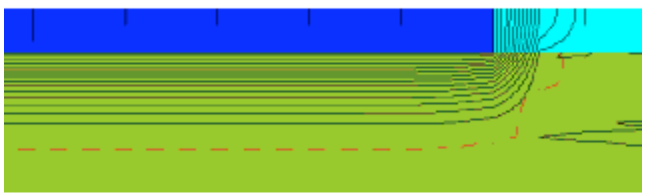
Energy Band Diagram

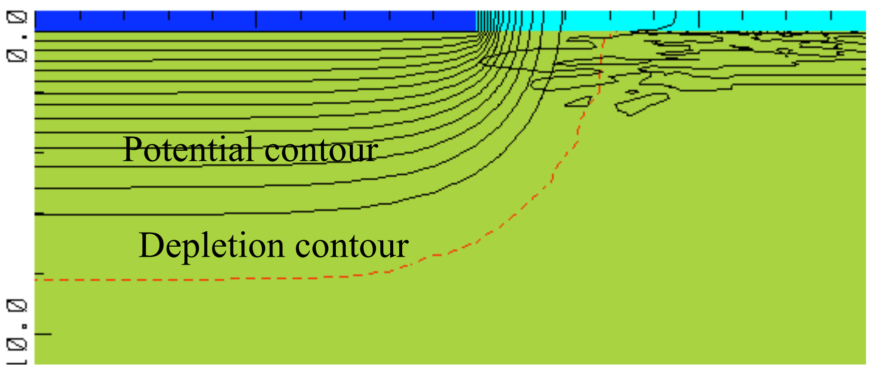


Sample IV curve

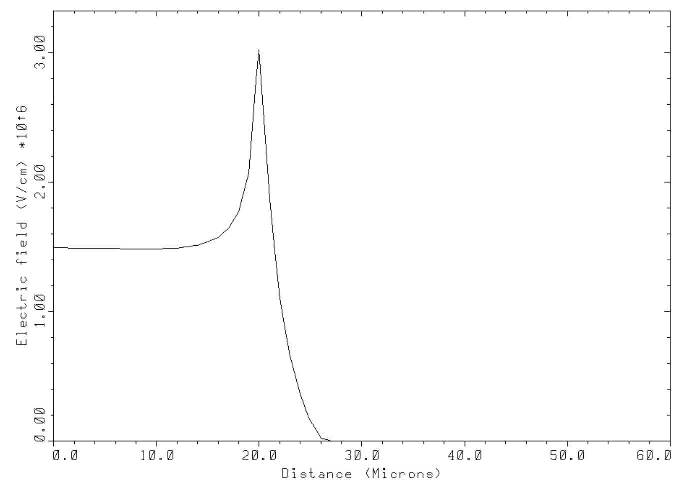
Edge Termination



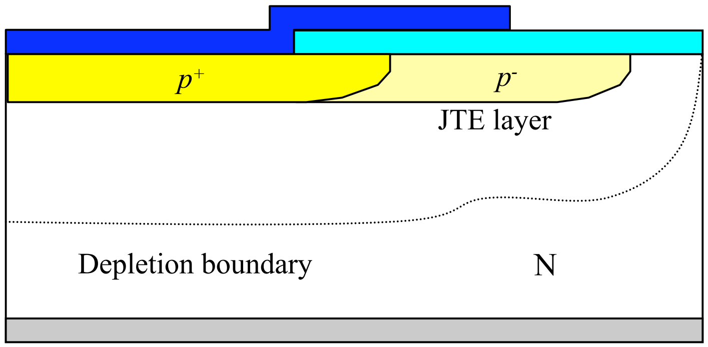




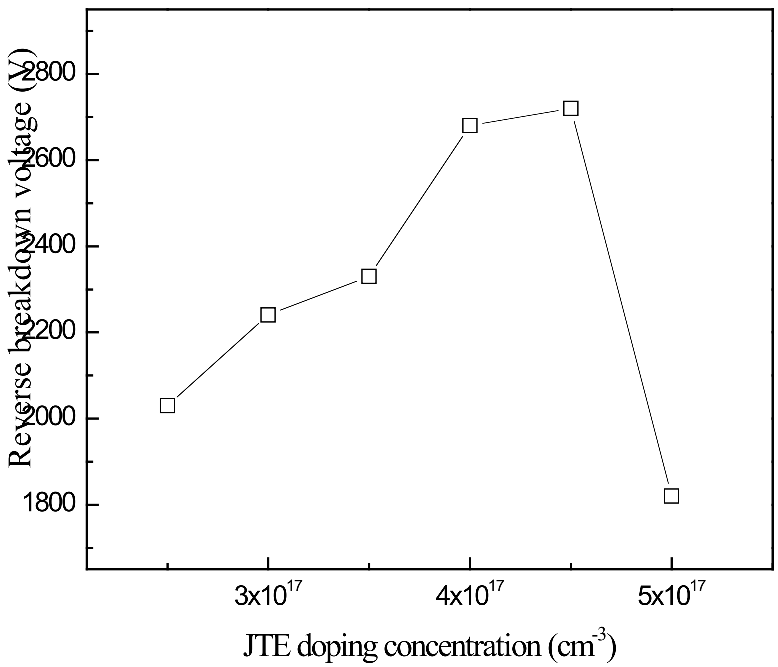
- Edge termination is critical for obtaining high breakdown voltage and reduced on-state resistance.
- Severe electric field crowding around metal contact periphery.
- High leakage current and breakdown at the highest electric field

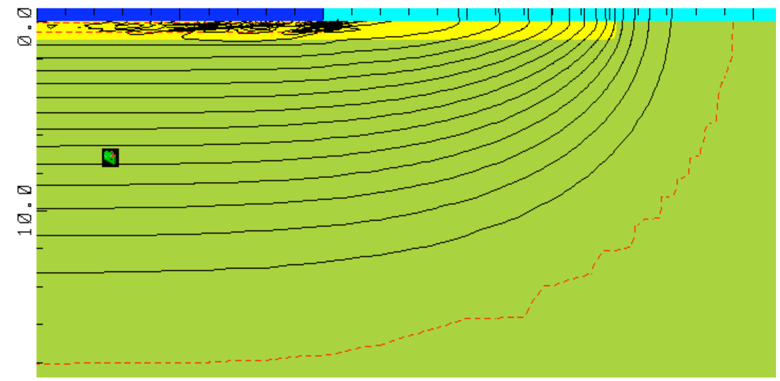


Junction Termination Extension



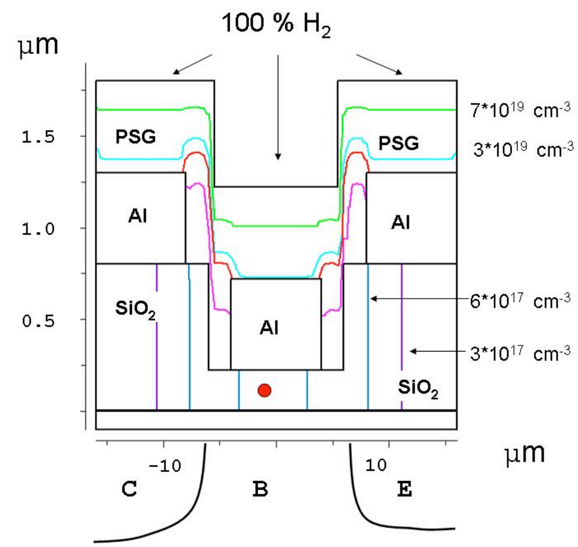
- V_B values are highly sensitive to the charge in the JTE layer.
- Multiple JTE termination technique (JTE1 + JTE2).





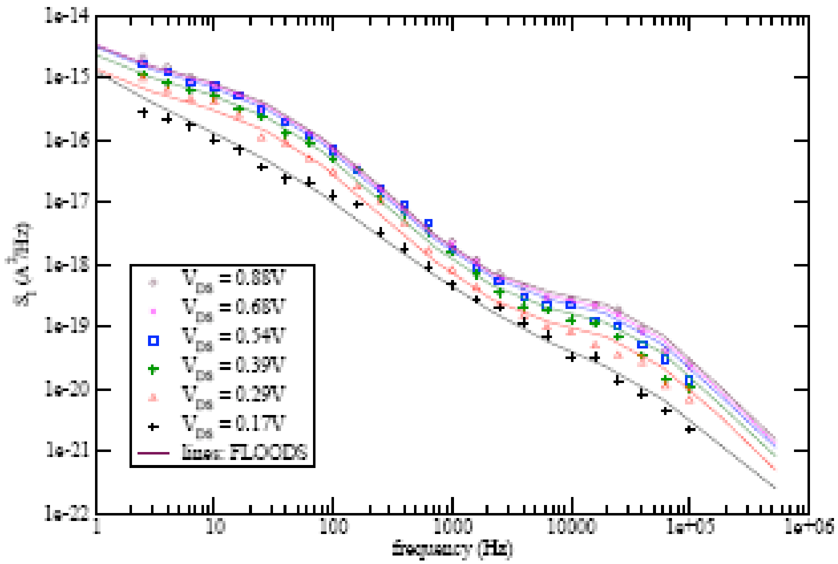
Reliability Simulation

- Simulate Device in Quasi-Steady State
  - Electrons and Holes equilibrate quickly
  - Similar to assumption in process simulation
- Generation Events Triggered by
  - Mechanical Stress
  - Current Flow / Electric Field
- Simultaneous solutions
  - Point Defects / Defect Cluster / Interface Capture
  - Hydrogen

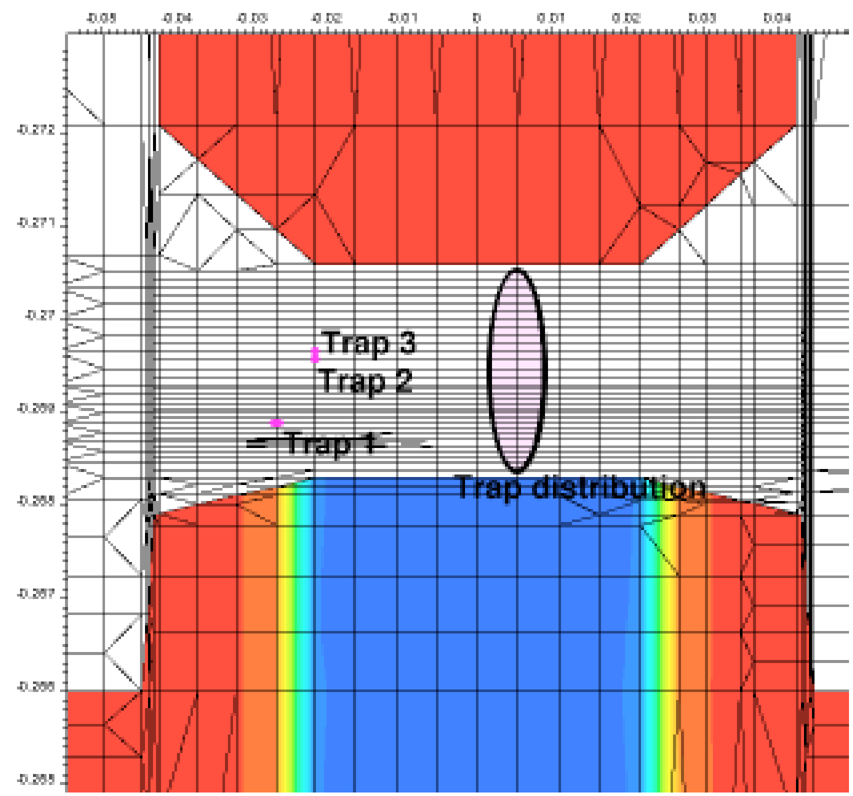


TNS, TBP
Vanderbilt
+ UF

Example: 3.2μm x 90nm bulk nMOSFET



Low frequency measured and simulated noise data



Graphical depiction of ***Noise Producing*** oxide trap locations on mesh for simulating the low frequency noise features. Location 1 has 4 traps, locations 2 and 3 0.5 traps each.

Conclusions

- Modeling Integrated
  - Fundamental Physics k•p feeds TCAD
  - Thermal coupled to TCAD
- Experimentally Integrated
  - Failure Mechanism Identification feeds M&S
  - Electrical Measurement feeds